

Supporting information

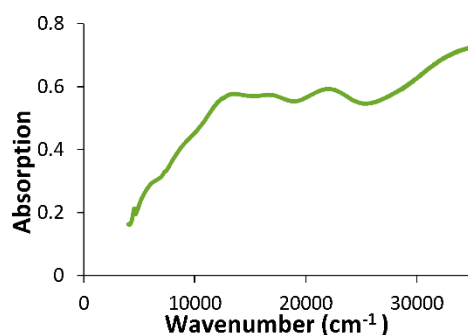
for

# Spectroscopic definition of the copper active sites in Mordenite : selective methane oxidation

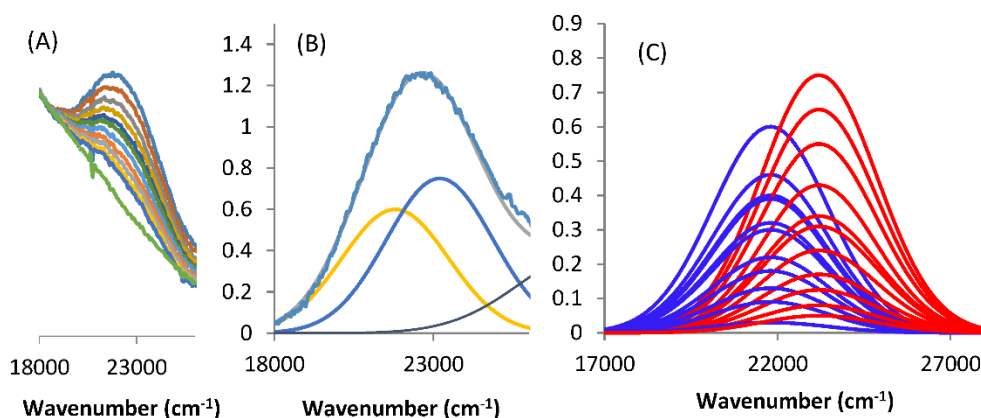
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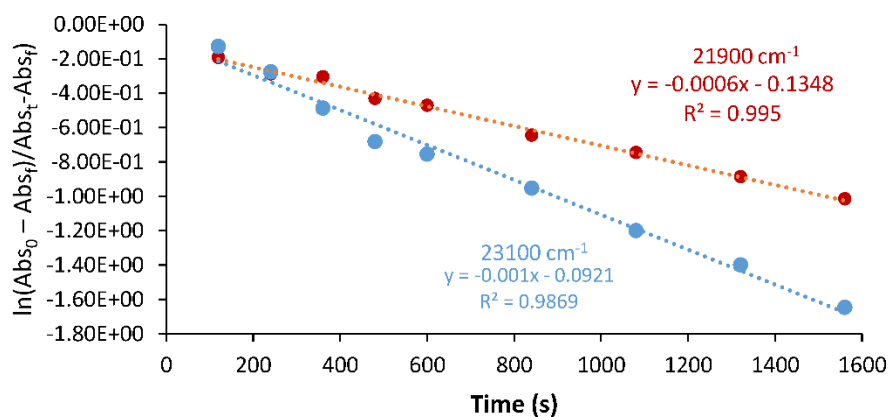
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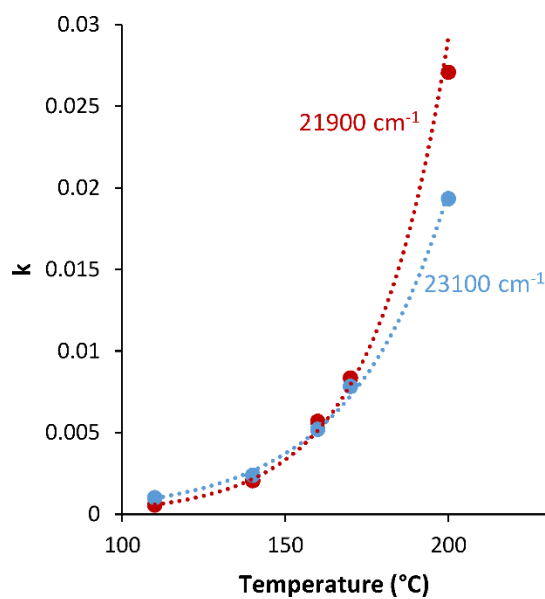
**Figure S1.** Cu-MOR sample after N<sub>2</sub>O activation



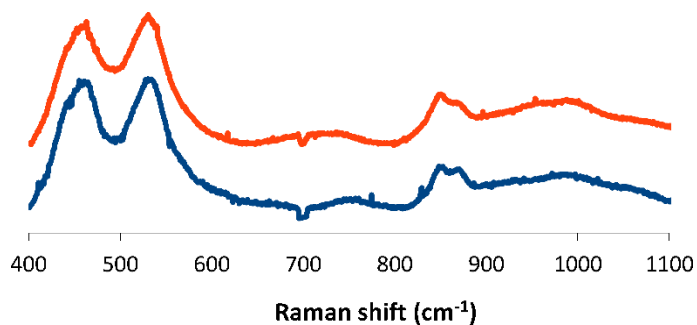
**Figure S2.** (A) Example of the disappearance of the 22200 cm<sup>-1</sup> band envelope during CH<sub>4</sub> reaction at 110°C; (B) Deconvolution of the absorption envelope at the start of the reaction. This is done for every spectrum that is measured in time. (C) The 21900 cm<sup>-1</sup> and 23100 cm<sup>-1</sup> absorption bands during CH<sub>4</sub> reaction at 110°C



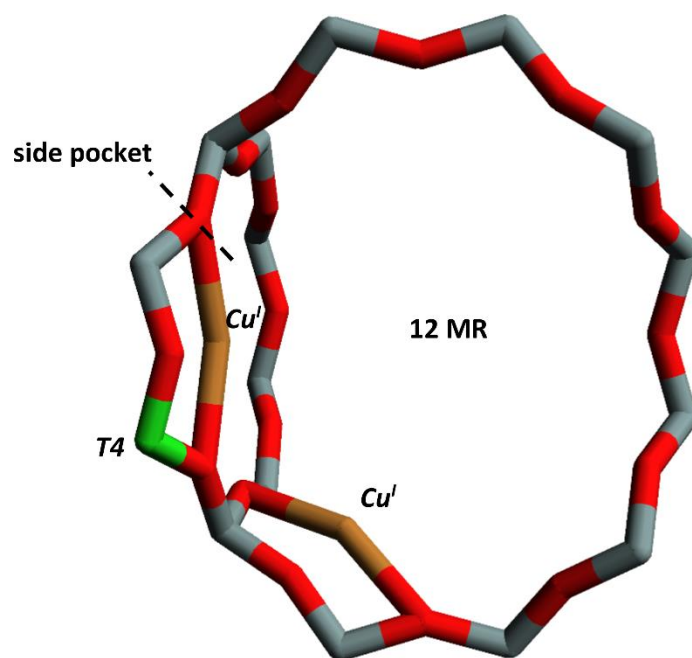
**Figure S3.** First order plots of the decay of the 21900 and 23100  $\text{cm}^{-1}$  bands at 110°C.



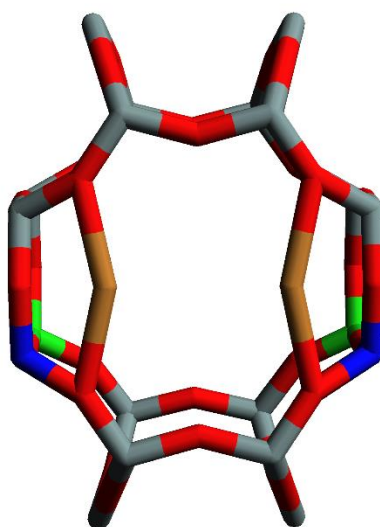
**Figure S4.** Comparison of the disappearance of the 21900 and 23100  $\text{cm}^{-1}$  bands during the  $\text{CH}_4$  reaction:  $k$  in function of the temperature.



**Figure S5.** Resonance Raman spectra ( $\lambda_{\text{ex}}=458 \text{ nm}$ ) of Cu-MOR activated with  $\text{O}_2$  (red) and  $\text{N}_2\text{O}$  (blue) at 250 °C.



**Figure S6.**  $\text{Cu}^{\text{I}}$  ions bound bidentate with bite angles of  $150^\circ$  can be placed at two positions (in yellow) in the 12 MR.



**Figure S7.** Pair of  $\text{Cu}^{\text{I}}$  atoms (yellow) with bite angles of  $150^\circ$  placed at two T3 sites (blue).